

Non-Monotone Characteristic of Spectral Statistics in the Transition between Poisson and Gauss

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Abstract

We have computed the spectral number variances of an extended random matrix ensemble predicted by Guhr's supersymmetry formula, showing a non-monotone increase of the curves that arises from an "overshoot" of the two-level correlation function above unity. On the basis of the most general form of N -level joint distribution that meets sound probabilistic conditions on matrix spaces, the above characteristic may be attributed to the *attractiveness* of the pair potential in long range ($E >$ Thouless energy) of the underlying level gas. The approach of level dynamics indicates that the result is "anti-screening" of the level repulsion in short-range statistics of the usual random matrix prediction until the joint level distribution undergoes a phase transition (the Anderson transition).

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There have been considerable efforts in solid-state and random matrix theories(RMT) to formalize metal-insulator transition phenomena as regards the pertinent electron energy level statistics, which seek a powerful and unified method to generalize the standard Gaussian ensembles initiated by Wigner, Dyson and Mehta [1] (see a comprehensive review on the recent development [2]).

Guhr has studied a method based on supersymmetry [3], and recently obtained a formula for computing the two-level correlation function $X_2(r)$ for a Hamiltonian system $H = H_0 + \alpha H_1$ with a parameter $\lambda(\lambda = \lambda(\alpha))$ to describe a transition from regularity to chaos [4,5]; $0 \leq \lambda \leq \infty$. It is assumed that $\lambda = 0$ (also $\alpha = 0$) represents the Poisson regularity for the system H_0 alone (which is subject to the Poisson statistics), and $\lambda = \infty$ the Gaussian unitary ensemble (GUE) for the system H_1 alone (which is subject to the GUE statistics). Namely, in Refs. [4,5], a double integration representation of the $X_2(r, \lambda)$ function is presented: the one involving a single Bessel function $J_1(z)$ [5] is shown to converge for $\lambda \rightarrow \infty$ to the well-known GUS correlation function $1 - \left(\frac{\sin \pi r}{\pi r}\right)^2$, and for the lowest non-zero term of the small λ

$$X_2(r, \lambda) = \frac{r}{\lambda} \int_0^\infty \exp(-k^2/2) \sin(rk/2) dk \quad (\text{valid for } \lambda \simeq 0.1 \text{ or smaller}). \quad (1)$$

Our concern in this report is not any inquiry about the supersymmetry basis of the formula nor its derivation, but a consequence of what Guhr called "overshoot" of the quantity $X_2(r, \lambda)$ above unity, i.e.

$$\text{a range of } r \text{ exists, where } X_2(r, \lambda) > 1. \quad (2)$$

This can best be visualized by plotting $X_2(r, \lambda)$ against r : here in Fig.1, we calculate four curves $\lambda = 0.1, 5, 10$ and ∞ , and compare them with the corresponding curves which are provided by another formula of Gaudin's model due to us [6] (Some feature of this model will be discussed later).

Since the unfolded scale is used always in the present formulas and figures (which also amounts to a change of the perturbation parameter α to λ), inequality (2) implies the negativeness of the corresponding cluster function $Y_2(r, \lambda)$ [1] so that

$$Y_2(r, \lambda) \equiv 1 - X_2(r, \lambda) < 0 \text{ in the same range.} \quad (2')$$

This causes a significant modification of the structure of the level statistics for such systems from the standard RMT. We would like to point out the following two remarks.

1. **Number variance curve** based on the well-known formula

$$\Sigma^2(s, \lambda) = s - 2 \int_0^s (s-r) Y_2(r, \lambda) dr. \quad (Y_2(-r, \lambda) = Y_2(r, \lambda).) \quad (3)$$

It can be seen readily from Eq.(3) that $\frac{d^2}{ds^2} \Sigma^2(s) = -Y_2(s) < 0$, which means that a $\Sigma^2(s)$ curve has an inflection point at the zero of Y_2 : more precisely, the increasing behavior of the curve changes its second derivative from minus to plus at the inflection point.

2. **N-level joint distribution** which we assume to be of the form

$$P(x_1, x_2, \dots, x_N) = \frac{1}{Z_\beta} \exp \left[-\beta \sum_{j < k} \phi(x_j - x_k) \right], \quad \beta = 1, 2 \text{ and } 4. \quad (4)$$

Here, the sum $\sum_{j < k} \phi(x_j - x_k)$ in the right hand side of eq.(4) to represent the interaction between the levels is common in most of extended RMT nowadays, and we shall state its axiomatic basis in **1st aspect** of Balian's strategy below.

The cluster expansion theory for imperfect classical gases in statistical mechanics tells us that, if the binary potential for a pair of the molecules is positive (i.e. everywhere repulsive), the second-order cluster function must be non-negative at least for the low density limit where it is approximated by the minus of the Mayer function, $1 - e^{-\beta\phi(r)}$ ($\beta > 0$) ([7] and a further account therein). Guhr's example of the smallest parameter value can be regarded as such a limiting situation so that the existence of the overshoot of Guhr's correlation function on the r -axis has a significance that, when the joint distribution of his model is expressed in the form of Eq.(4), the potential ϕ for a pair of levels x_j and x_k must have an attractive portion somewhere in the configuration space (x_j, x_k) of the levels. *Does this mean a level attraction rather than the level repulsion of the standard RMT sense?*

The possibility of long-range level attraction has been discussed by Jalabert, Pichard and Beenakker [8] for actual disordered metals. We shall discuss this question, referring to another recent paper by Weinmann and Pichard [9] who observed the behavior of non-monotone increase of the number-variance curves in a selected actual matrix ensemble and analyzed the data on their advocacy of "Gaussian matrix ensemble with preferential basis" (cf. [10]). Before going, we present a numerical and graphical confirmation of the non-monotone behaviors of the theoretical Σ^2 curves predicted by Guhr's formula (1) and that from a related approximation (see Eq. (4.3) in Ref. [11]).

As can be seen in Fig.2(a), the non-monotone characteristic is common for all the parameter values, although the overshoot becomes obscure in Fig.1(a) quickly as λ increases. So, it is important to fix the range of λ on which the non-monotone character remains to exist, in particular, to ask its existence for large λ 's. The latter question has been answered affirmatively by Fram, Guhr, and Müller-Groeling [11], who have provided a numerically tractable formula to replace Eq.(1) for $X_2(r, \lambda)$. Moreover, they have shown a further simplification of the formula which turns out to be a divergent perturbation (i.e. starting from $\lambda = \infty$) by which $\Sigma^2(s)$ for $\lambda \gg 1$ can be understood easily.

Leaving the actual graphs of confirmation to the paper [11], we argue the existence of overshoot for $\lambda \gg 1$ by means of their reduced formula:

$$X_2(r, \lambda) = X_2^{GUE}(r) + X_2^{(1)}(r, \lambda) + X_2^{(2)}(r, \lambda) + (\text{correction}),$$

where the term (correction) vanishes faster than r^{-2} for $r \rightarrow \infty$. In terms of the cluster function $Y_2(r, \lambda)$ with neglect of such corrections,

$$Y_2(r, \lambda) = \left(\frac{\sin \pi r}{\pi r} \right)^2 - X_2^{(1)}(r, \lambda) - X_2^{(2)}(r, \lambda), \quad (5)$$

where

$$X_2^{(1)}(r, \lambda) = \frac{1}{\pi} \frac{\pi \lambda^2}{(\pi \lambda^2)^2 + r^2}, \quad \int_{-\infty}^{\infty} X_2^{(1)}(r, \lambda) dr = 1, \quad (5a)$$

and

$$X_2^{(2)}(r, \lambda) = \frac{1}{2\pi^2} \frac{r^2 - (\pi \lambda^2)^2}{((\pi \lambda^2)^2 + r^2)^2}, \quad \int_{-\infty}^{\infty} X_2^{(2)}(r, \lambda) dr = 0. \quad (5b)$$

It shows that the first-order correction $X_2^{(1)}$ (Breit-Wigner term) compensates the familiar GUE part, together with the second-order correction $X_2^{(2)}$ contributing negatively to the cluster function for almost all r values ($|r| > r_0$ with some small r_0), which confirms the negativeness of $Y_2(r, \lambda)$ above the r_0 . At the same time, $\int_{-\infty}^{+\infty} Y_2(r, \lambda) dr = 0$ for almost all λ values, indicating that the Σ^2 curve approaches an asymptotic straight line that is the pure Poisson with no deviation of the coefficient from unity. The feature quite differs from the counter example of Gaudin's model [6], as exhibited in Fig.2(b).

To be a significance in the above two works, the authors of [9] and [11] have presented actual matrix ensembles which display, as computer experimental results, the non-monotone number-variances: this stimulates us to construct an adequate statistical model capable of a unified description of both types; the monotone type and the non-monotone type. So, let us examine the concept of Gaussian matrix ensemble with preferential basis of Refs. [9,10].

Our conclusion is precedently stated: the formulation as it stands is not capable of describing the non-monotone characteristic, because their potential function ϕ is everywhere positive, as exemplified by Eq.(11) of Ref. [10] that is identical to [6] for Fig.2(b). However, this formulation can be revised without loss of sound mathematical basis to include the non-monotone characteristic, which we will discuss in the rest of the present report.

There are two aspects of the *Gaussian matrix ensemble with preferential basis* to be reexamined seriously, in order to allow it with the possibility of attractiveness of the pair potential: the first is a proper introduction of the *preferential basis*, and the second, a right way of setting up constraints in *maximum entropy principle* for the Gaussian probability density function. Both aspects are combined to give the most efficient realization of Balian's strategy [12].

1st aspect. An element of Balian's strategy in RMT is an introduction of Riemannian metrics on matrix spaces in the form $\text{Tr} dM dM^*$ by which an information quantity is written (his *postulate A*). This is particularly relevant in the present problem, because a fixing of the metric tensor is the starting point of the whole subject of a Gaussian probability that is an exponential of the metric form. Namely,

$$P(A) = C \exp\left[-\frac{1}{2} K(A, A)\right], \quad K(A, A) = \sum_{\alpha, \beta} K_{\alpha, \beta} A_{\alpha}^* A_{\beta} \geq 0 \quad (\text{equality only } A = 0), \quad (6)$$

where A_{α} is a tangent vector component of the metric form as the Gaussian random variable. We then ask what is the most general metric form defined on matrix spaces (See a detailed discussion [13]). The answer is given by a *covariant bilinear form* of any two $N \times N$ hermitian(or, unitary) matrices A and B depending on another hermitian matrix H to satisfy *representation invariance* all together. It is expressed as

$$K_H(B, A) = \text{ReTr} B^* C_H(A), \quad (7)$$

in terms of a linear superoperator C_H on A , and satisfies the covariance condition

$$K_{U^* H U}(U^* B U, U^* A U) = K_H(B, A) \quad \text{for any unitary } U \in G_{\beta}, \quad (7a)$$

where G_{β} is the symmetry group associated with β . An adequate choice of the representation is naturally the H -diagonal representation ($H_D = \text{diag}(x_1, \dots, x_N)$ by a choice of U to diagonalize H) that yields *preferential basis*: by this choice we can rewrite (7) as

$$K_H(A, A) = \sum_j c(x_j) |A_{jj}|^2 + 2 \sum_{j < k} f(x_j, x_k) |A_{jk}|^2 \quad \text{with real positive } c(x), f(x, y) \quad (8)$$

$$\text{and} \quad f(x, y) = f(y, x). \quad (8a)$$

By definition of the trace operation in eq.(7), there is no actual priority of the representation basis in our "preferential basis", as it were supposed by the saying "*H*-diagonal representation" that might sound a kind of symmetry break[10] to prohibit some $U \in G_\beta$. Instead, the unitary covariance (7a) allows U to cover the full group G_β so that the Gaussian variables $\{A_{jk}\}$ are decorrelated from $\{x_j\}$, and upon being integrated over these variables, the resulting reduced probability density function depends on the eigenvalue indices only through $\{x_j\}$ that are mutually fully equivalent to each other(so-called *identically distributed*). Another characteristic of the Gaussian probability function (6), when the form (7) is inserted (with $\alpha = jk$), is the *statistical independence* of A_α 's; the fact that the metric tensor in the form(8) is diagonal with respect to α . Let us further impose the third condition of *translational invariance*($x_j \rightarrow x_j + x$ makes the metric tensor unchanged). Then, the form (8) is further simplified such that a single function $f(x - y)$ is enough to characterize the N -level joint probability function $P(x_1, \dots, x_N)$ as in the form (4). (This is seen by the integration of the function (6) over the *cotangent* variables defined by $\tilde{A}_{jk} = 2f(x_j - x_k)A_{jk}$.) We then get

$$\phi(r) = -\frac{1}{2} \log f(r) = \frac{1}{2} \log \frac{1}{f(r)}. \quad (9)$$

This is because the result of the integrations is expressed as the square-root of the determinant of the metric tensor that yields $P(x_1, \dots, x_N)$. At the same time, a probabilistic meaning of the function $f(x_j - x_k)$ is assigned to be the variance of the Gaussian cotangent variable \tilde{A}_{jk} (or, its each component, if it is complex, and quaternion depending on the multiplicity $\beta = 2$, and 4, respectively). To summarize, we can say

the most general expression for N -joint level distribution P_N as an integral reduction of the Gaussian form (6) satisfying the identicalness, statistical independence and translational invariance must be the form (4). (An inclusion of one-level potentials is another matter.)

2nd aspect. It is important to remark that, in order to apply the maximum entropy principle to assign a form to the probability function $P(\tilde{A})$ (Balian's *postulate B*), a Gaussian probability has a special property of its entropy. Namely, the Gaussian probability function $P_G(\tilde{A}_{jk})$ with the variance $f(x_j - x_k)$ is characterized by the maximum entropy of all the probability functions with the same variance, thus denoting the entropy functional of $P, \langle -\log P \rangle_P$, by $H[P]$, we can express this fact as

$$\max_P H[P] = H[P_G] \quad \text{under constraint } \text{Var}(\tilde{A}_{jk}) = f(x_j - x_k). \quad (10)$$

(For the legitimacy of a maximum entropy principle with non-constant constraint, see [14].) It tells us that the variance (10) must be the right quantity of constraint for the present maximization problem. Therefore, without any further information about the matrix ensemble, we have no criterion about the degree of attractiveness of the pair potential ϕ that is only related to the form of variance f as Eq.(9): all what is needed is the positivity $f > 0$.

However, a powerful information can be provided by *level dynamics* [6](cf.[14]), where it is shown that, if the diagonalization process of a hermitian matrix H (or, its unitarization $U_0 e^{iH}$) is put into a Hamiltonian dynamics, a possible equilibrium state of this dynamical system can be selected by the above maximization as a one-parameter family of canonical distributions (in the sense of statistical mechanics of Hamiltonian systems) and represented by the form

$$P_G(\tilde{A}) \propto \prod_{j < k} \exp \left[-\frac{1}{2f(x_j - x_k)} |\tilde{A}_{jk}|^2 \right], \quad \text{with } f(r) = \left| \frac{\mu r^2}{1 + \mu r^2} \right| \text{ (hermitian case),} \quad (11)$$

and hence

$$\phi(r) = \frac{1}{2} \log \left| 1 + \frac{1}{\mu r^2} \right|. \quad (11a)$$

A positive parameter value μ corresponds to Gaudin's linear-gas model [15], also identical to the formula of Refs. [9,10] for which ϕ is fully repulsive. To our emphasis, however, there is no *a priori* reason to restrict us to the positivity of μ (as far as $f(r)$ is retained as positive), and let us look at the possibility of choosing a *negative* μ (This amounts to a sign change of Yukawa's parameter γ [16]): it makes the potential ϕ partially attractive such that

$$\phi(r) = \frac{1}{2} \log \left(\frac{1}{|\mu| r^2} - 1 \right) \quad |r| < 1/\sqrt{|\mu|}; \quad \frac{1}{2} \log \left(1 - \frac{1}{|\mu| r^2} \right) \quad |r| > 1/\sqrt{|\mu|},$$

with the attractive range $1/\sqrt{2|\mu|} < |r| < \infty$, (12)

and at the same time, for small values of the level distance including the repulsive range ($|r| < 1/\sqrt{2|\mu|}$),

$$f(r) = r^2 |\mu| / (1 - |\mu| r^2) \quad |r| < 1/\sqrt{|\mu|}. \quad (13)$$

(A schematic behavior of the entire potential function $\phi(r)$ can be seen in Fig.3.) This can be interpreted as an *anti-screening* of the level repulsion in short-range rather than the screening assigned to it in Gaudin's model by the original proposal [10], and as the actual level attraction in the range specified by (12) for long-range level statistics.

There exist two routes of the Wigner-Dyson Gaussian standard of electron energy level statistics to Poisson regularity; one $\mu(=0)$ tends to infinity on the positive axis, and the other $\mu(=0)$ to infinity on the negative axis, and it is remarkable that the latter route undergoes a singularity of the level distribution that can well be assigned to be the Anderson transition with Thouless energy $E_c = \Delta/\sqrt{|\mu|}$ (Δ is the average spacing in energy scale): the resulting Poisson statistics must be on localized electrons that, at the same time, give rise to a real symmetry-breaking of the representation (the metric tensor then depends on the indices jk as $e^{-\alpha|j-k|}$). Existence of both repulsive and attractive inter-level pair-wise interaction was first indicated by [8] for disordered metals, and from the present viewpoint these provide a distinction between absence and presence of the transition, and it can be tested by the monotonicity or non-monotonicity in the number-variance curve as in Fig.2.

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FIGURES

Fig 1

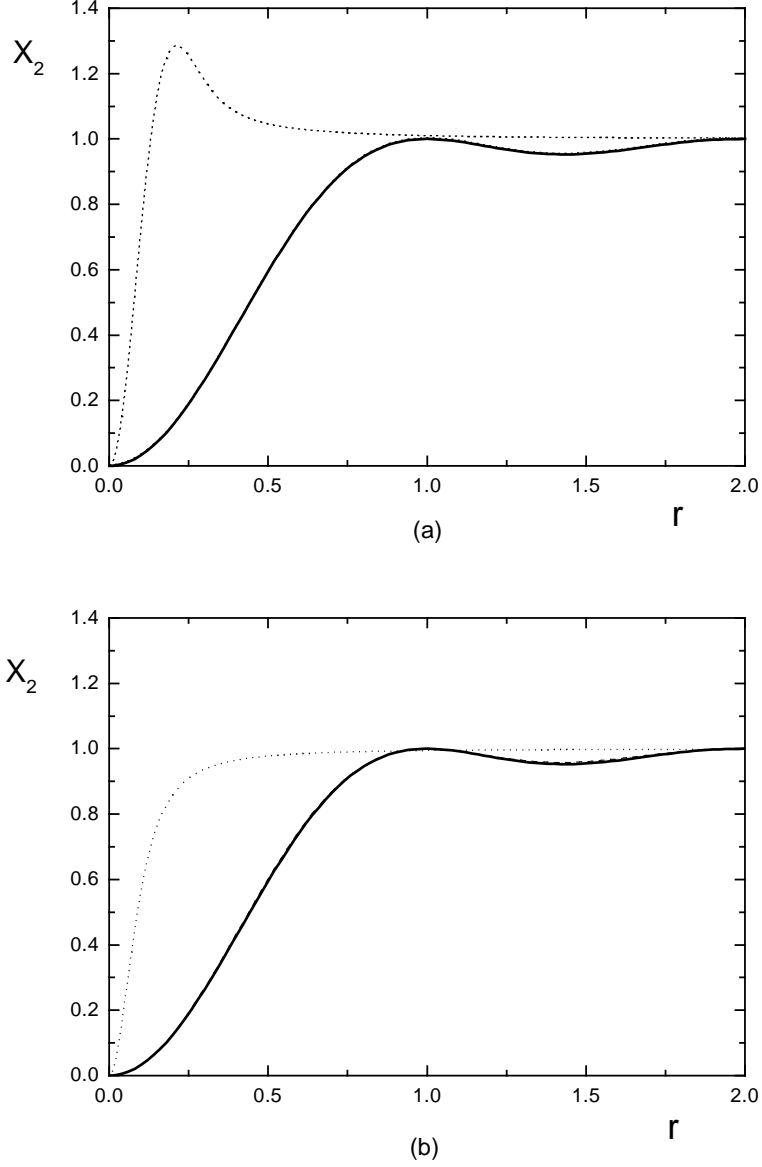


FIG. 1. $X_2(r, \lambda)$ for different values of the transition parameter λ from two different theories. (a) Calculated from Guhr's formula for $\lambda \ll 1$ and $\pi\lambda^2 \gg 1$. (b) Calculated from Gaudin's model (Eqs. (4.5) of Ref. [6]) From the left to right the curves correspond to $\lambda = 0.1, 5, 10$ and ∞ . The curves of $\lambda = 5$ and 10 are almost indistinguishable from the GUE curve (solid line).

Fig 2

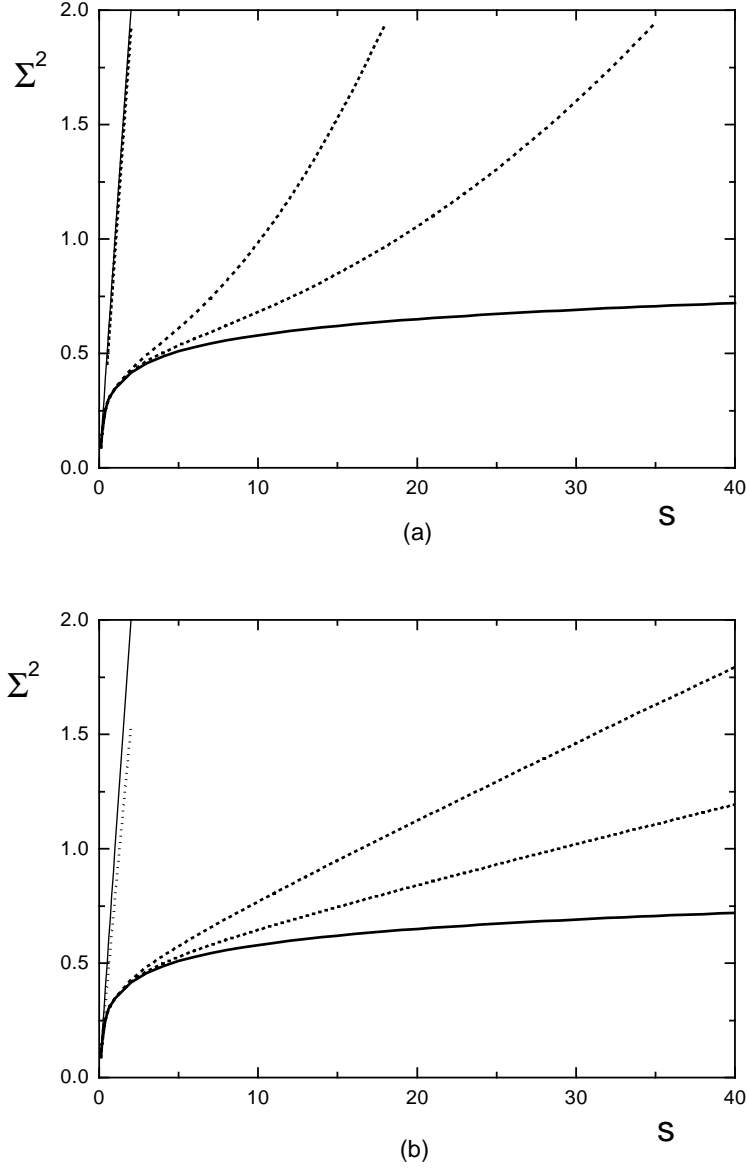


FIG. 2. Number variance $\Sigma^2(s, \lambda)$ for two different models. (a) From Guhr's model (Eq. (4.4) of Ref. [10]). (b) From Gaudin's model due to Hasegawa and Ma [6]. The non-monotonic behavior in (a) is very obvious. From the left to right the curves correspond to the Poisson, $\lambda = 0.1, 5, 10$ and ∞ (GUE), respectively.

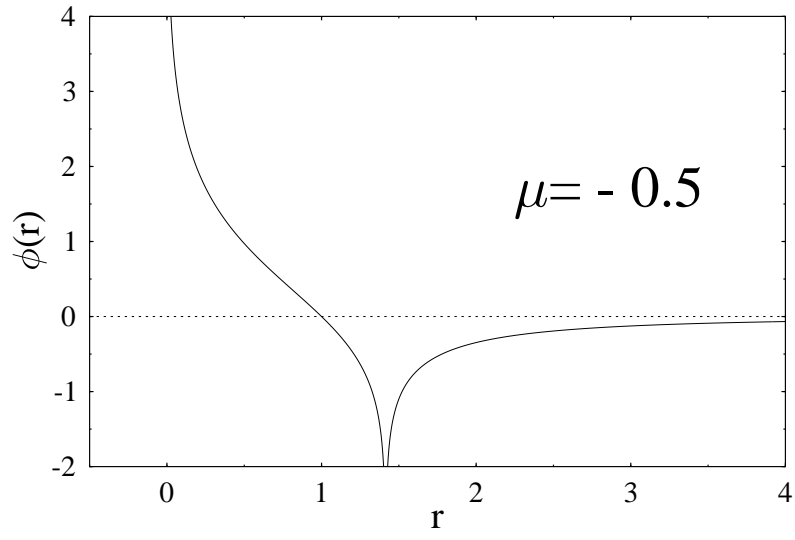


FIG. 3. $\phi(r)$ vs r for $\mu = -0.5$ given by Eq. (11a).